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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
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10/526,335

11/16/2005

Tim Cheeseright

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EXAMINER

SKOWRONEK, KARLHEINZ R

ART UNIT

PAPER NUMBER

1631

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PAPER

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

<b>Office Action Summary</b>	<b>Application No.</b> 10/526,335	<b>Applicant(s)</b> CHEESERIGHT ET AL.	
	<b>Examiner</b> KARLHEINZ R. SKOWRONEK	<b>Art Unit</b> 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

### Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

### Status

- 1) ☒ Responsive to communication(s) filed on 05 June 2009.
- 2a) ☐ This action is **FINAL**.                      2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

### Disposition of Claims

- 4) ☒ Claim(s) 1-13 and 16 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☐ Claim(s) 1-13 and 16 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

### Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on \_\_\_\_\_ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.  
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

### Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All    b) ☐ Some \*    c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
  2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
  3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

\* See the attached detailed Office action for a list of the certified copies not received.

### Attachment(s)

- |  |   |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892)          | 4) <input type="checkbox"/> Interview Summary (PTO-413)           |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____                                      |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08)          | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date _____  | 6) <input type="checkbox"/> Other: _____                          |

## **DETAILED ACTION**

### ***Continued Examination Under 37 CFR 1.114***

A request for continued examination under 37 CFR 1.114 was filed in this application after appeal to the Board of Patent Appeals and Interferences, but prior to a decision on the appeal. Since this application is eligible for continued examination under 37 CFR 1.114 and the fee set forth in 37 CFR 1.17(e) has been timely paid, the appeal has been withdrawn pursuant to 37 CFR 1.114 and prosecution in this application has been reopened pursuant to 37 CFR 1.114. Applicant's submission filed on 05 June 2009 has been entered.

### ***Claim Status***

Claims 1-13 and 16 are pending.

Claims 14-15 are cancelled.

Claims 1-13 and 16 have been examined.

Claims 1-13 and 16 are rejected.

### ***Priority***

This application was filed on 16 November 2005 and is the 35 USC 371 National phase application of International Application PCT/GB03/03605 filed on 18 August 2003.

### ***Claim Rejections - 35 USC § 101***

#### ***Response to Arguments***

The rejection of claim 13 as directed to non-statutory subject matter under 35 USC 101 is withdrawn in view of applicant's argument in the response filed that a computer interpretable recording medium is not a carrier signal.

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

The following rejection is maintained from the previous action.

Claims 1-12 and 16 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

Claims 1-12 are directed to a process for identifying candidate molecules by comparison of molecular fields. The following analysis is taken from the guidance provided in the MPEP at 2104.IV, "Determine Whether the Claimed Invention Complies with 35 USC101". The claims are directed to processes. Here the claims are directed to the abstract idea of quantifying the similarity between two molecules by comparing derived mathematical predictions of the fields representing the molecules. The processes do not recite a physical transformation of matter from one state to another. Giving the claims the broadest reasonable interpretation, the claims read on mental steps. In *Comiskey* (*In re Comiskey*, 84 USPQ2d 1670) the court established that "the application of human intelligence to the solution of practical problems is not and of itself patentable" (at 1680). In *Comiskey*, the court stated explicitly "mental processes - or processes of human thinking - standing alone are not patentable even if they have a practical application" (at 1679). The court in *Comiskey* stated, "Following the lead of the Supreme Court, this court and our predecessor court have refused to find processes

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patentable when they merely claimed a mental process standing alone and untied to another category of statutory subject matter even when a practical application was claimed” (at 1680). The court’s recent decision in *In re Bilski* confirmed, “a process is patent-eligible under 35 USC 101 if it is tied to a particular machine or apparatus or if it transforms a particular article into a different state or thing” (*In re Bilski*, 88 USPQ at 1391, 2008). In the instant claims, the process is not tied to a class of statutory invention. Claims 1-12 recite providing an output or a response to a user. The output is insignificant post-solution activity and does not represent a significant tie to another category of invention. The court in *Comiskey*, stated, “the court rejected the notion that mere recitation of a practical application of an abstract idea makes it patentable, concluding that ‘[a] competent draftsman could attach some form of post-solution activity to almost any mathematical formula’” citing *Flook* (437 U.S. at 586, 590). The recent decision in *Bilski* confirmed the court’s position regarding insignificant pre- or post-solution activity (i.e. insignificant extra-solution activity) as stated in *Comiskey* (see *In re Bilski*, 88 USPQ2d 1385 (Fed. Cir. 2008) at p. 13-96-1397). Applicant is encouraged to consider the recent BPAI informative decisions *Exparte Langemyr* (No. 2008-1495 (28 May 2008)) and *Exparte Biliski* (No. 2002-2257 (26 September 2006)) for further clarification of the above grounds of rejection.

### ***Response to Arguments***

Applicant's arguments filed 05 June 2009 have been fully considered but they are not persuasive. Applicant argues the claims as amended transform field point data into a score and thus satisfies the machine or transform test put forth by the CAFC in the *In*

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*re Bilski* decision. The argument is not persuasive. The claims are directed to the mathematical manipulation of data from one form to another. The court in *Bilski* indicated rather clearly that a patent eligible transformation “transforms a particular article into a different state or thing” (*In re Bilski*, 88 USPQ at 1391, 2008). In the instant case, no such transformation is taking place. The rejection is maintained

The following rejection is new.

Claim 16 is directed to a computer apparatus. A review of the specification reveals the following description of a computer apparatus, “The computer apparatus may be configured in hardware, firmware, or software, or in a combination thereof” (p. 9 lines 23-24). Thus, an embodiment of the instantly claimed computer apparatus is a program *per se*. The MPEP, at 2106.01, guides that computer programs *per se* are non-statutory. The claim is directed a program *per se* and are non-statutory.

### ***Claim Rejections - 35 USC § 112***

The following is a quotation of the second paragraph of 35 U.S.C. 112:

The specification shall conclude with one or more claims particularly pointing out and distinctly claiming the subject matter which the applicant regards as his invention.

The following rejection is new as necessitated by amendment of the claims.

Claim 1-13 and 16 is rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

Claim 1 provides for the use of the score to identify potential candidates in line 11-12, but, since the claim does not set forth any steps involved in the method/process, it is unclear what method/process applicant is intending to encompass. A claim is indefinite where it merely recites a use without any active, positive steps delimiting how this use is actually practiced. Claim 1 is further unclear with respect to what is being identified in the employing step. The metes and bounds of the claim are rendered indefinite because all second molecules are potential candidates by nature of the comparison. Thus, it is unclear what applicant intends to claim in the employing step. If applicant intended the claim to encompass a step of providing a measure of the second molecule to have the known biological or physicochemical activity of the first molecule then an amendment to such would be appropriate. Claims 2-13 and 16 are also rejected because they depend from claim 1, and thus contain the above issues due to said dependence.

Claim 1 is rejected under 35 U.S.C. 101 because the claimed recitation of a use, without setting forth any steps involved in the process, results in an improper definition of a process, i.e., results in a claim which is not a proper process claim under 35 U.S.C. 101. See for example *Ex parte Dunki*, 153 USPQ 678 (Bd.App. 1967) and *Clinical Products, Ltd. v. Brenner*, 255 F. Supp. 131, 149 USPQ 475 (D.D.C. 1966).

### ***Claim Rejections - 35 USC § 103***

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

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(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

This application currently names joint inventors. In considering patentability of the claims under 35 U.S.C. 103(a), the examiner presumes that the subject matter of the various claims was commonly owned at the time any inventions covered therein were made absent any evidence to the contrary. Applicant is advised of the obligation under 37 CFR 1.56 to point out the inventor and invention dates of each claim that was not commonly owned at the time a later invention was made in order for the examiner to consider the applicability of 35 U.S.C. 103(c) and potential 35 U.S.C. 102(e), (f) or (g) prior art under 35 U.S.C. 103(a).

The factual inquiries set forth in *Graham v. John Deere Co.*, 383 U.S. 1, 148 USPQ 459 (1966), that are applied for establishing a background for determining obviousness under 35 U.S.C. 103(a) are summarized as follows:

1. Determining the scope and contents of the prior art.
2. Ascertaining the differences between the prior art and the claims at issue.
3. Resolving the level of ordinary skill in the pertinent art.
4. Considering objective evidence present in the application indicating obviousness or nonobviousness.

The following rejection is new.

Claims 1-3, 6, 11-13, and 16 are rejected under 35 U.S.C. 103(a) as being unpatentable over Mestres et al. (J. Molecular Graphics and Modeling, Vol. 15, p. 114-121, 1997) in view of Vinter et al. (IDS ref #1, filed 11/16/2005) and in view of Apaya et al. (IDS ref #2, filed 11/16/2005).



The claims are directed to a method of comparing molecules in which a set of field points representing field extrema, having a position and a field size, for a first molecule are provided; determining a field for second molecule at the field point position of the first molecule to obtain field sample values; compare the field sample values with the field size values to provide a score indicative of field similarity between the molecules; and identify the second molecule as a candidate from the score. Claim 13 is directed to a computer readable recording medium. Claim 16 is directed to a computational system. Claim 2 is directed to an embodiment in which field size values are determined from a field definition formula. Claim 3 is directed to an embodiment in which field size values are calculated from the interpolation of a grid. Claim 6 is directed to an embodiment in which the product between the field sample values and the field size values is determined. Claim 11 is directed to an embodiment in which the field size values are energy values. Claim 12 is directed to an embodiment in which the extrema are minima.

Mestres et al. shows that in molecular field similarity comparisons indices can be evaluated for specific points in grid embedding the molecules compared (p. 115, col. 2). Mestres et al. shows that for each position in the field of the first molecules the field of the second molecule is determined (p. 115, col. 2). Mestres et al. shows the score is used for identifying potential candidates that mimic the first molecule (p. 117, col. 1). Mestres et al. shows the product between the field sample values and the field size values is determined (eqn 3). Mestres et al. shows a computer readable recording

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medium and computational system (p. 115, col. 1). Mestres et al. shows the calculation of field size values from an interpolation of a grid (p. 117, col. 1-2).

Mestres does not show a set of field points representing field extrema.

Vinter et al. shows the calculation of a set of field points that represents the extrema of a molecule having a position and a field size value (p. 299, col. 2). Vinter et al. shows that the field extrema for a can be compared to the field of another molecule (p. 301, col. 1). Vinter et al. shows field size values are calculated from a field definition formula (p. 229, col. 1-2). Vinter et al. shows that field size values are energy values (p. 299, col. 2). Vinter et al. shows an advantage of comparing field extrema is the simplification of the energy map determination (abstract). Vinter et al. shows extrema are minima (p. 300, col. 1).

Apaya et al. shows the matching of extrema is more apparent using the accurate electrostatic models than it was when this approach was first applied, using semi-empirical point charge models (abstract). Apaya et al. shows that by optimizing the overlay of electrostatic extrema it is possible to identify an overlay that has a plausible binding orientation (p. 42, col. 2).

It would have been obvious to one of ordinary skill in the art at the time of invention to modify the method of molecular field comparison of Mestres et al. with the positions and field extrema of Vintner et al. and Apaya et al. because Vintner et al. shows an advantage of comparing field extrema is the simplification of the energy map determination and Apaya et al. shows that by optimizing the overlay of electrostatic extrema it is possible to identify an overlay that has a plausible binding orientation.

The following rejection is new.

Claims 7-10 are rejected under 35 U.S.C. 103(a) as being unpatentable over Mestres et al. in view of Vinter et al. and in view of Apaya et al. as applied to claims 1-3, 6, 11-13, and 16 above, and further in view of Maggoria et al. (Journal of Mathematical Chemistry Vol. 31, No. 3, April 2002).

Claim 7 is directed to the determination of an aggregate score. Claim 9 is directed to an embodiment in which field size values are calculated from the interpolation of a grid. Claim 8 is directed to an embodiment in which field size values are determined from a field definition formula. Claim 10 is directed to an embodiment in which the product between the field sample values and the field size values is determined.

Mestres et al. in view of Vinter et al. and in view of Apaya et al. as applied to claims 1-3, 6, 11-13, and 16 above shows a method of comparing the field extrema of a molecule to the field of another molecule to produce a similarity score. With respect to claim 8, Vinter shows field size values are calculated from a field definition formula (p. 229, col. 1-2). With respect to claim 9, Mestres et al. shows the calculation of field size values from an interpolation of a grid (p. 117, col. 1-2). With respect to claim 10, Mestres et al. shows the product between the field sample values and the field size values is determined (eqn 3).

Mestres et al. in view of Vinter et al. and in view of Apaya et al. do not show an the determination of an aggregate score.

Maggoria et al. shows the determination of an aggregate score (p. 254).  
Maggoria et al. shows that aggregate scores establish a foundation for a better understanding of the qualitative and quantitative aspects of field-based molecular similarity, and provides a means for a numerical characterization of the relative performance of various field-based similarity indices (p. 267).

It would have been obvious to one of ordinary skill in the art at the time of invention to modify the method for comparing the field extrema of a molecule to the field of another molecule to produce a similarity score of Mestres et al. in view of Vinter et al. and in view of Apaya et al. as applied to claims 1-3, 6, 11-13, and 16 above with the determination of an aggregate score of Maggoria et al. because Maggoria et al. shows that aggregate scores establish a foundation for a better understanding of the qualitative and quantitative aspects of field-based molecular similarity, and provides a means for a numerical characterization of the relative performance of various field-based similarity indices.

### ***Conclusion***

Any inquiry concerning this communication or earlier communications from the examiner should be directed to KARLHEINZ R. SKOWRONEK whose telephone number is (571)272-9047. The examiner can normally be reached on 8:00am-5:00pm Monday-Friday.

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If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran can be reached on (571) 272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/KARLHEINZ R SKOWRONEK/

Examiner, Art Unit 1631

5 August 2009

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